Simulation of Mass Transfer in a Microfluidic Experiment Using the Moving Mesh Method

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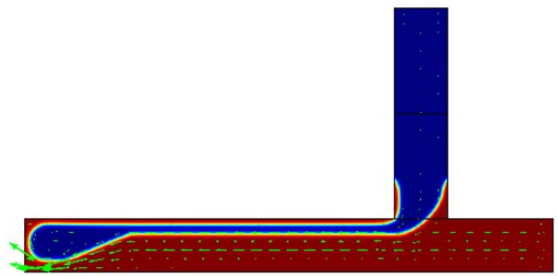
Modeling of Microreactors

- Two phase liquid-liquid systems are used extensively in chemical processes
- Microfluidics promises high mass transfer rates and compactness
- Optimization of a microreactor system must address numerous configuration options and operating parameters
- Progress has been made toward characterization of two-phase flow
- Need a definitive set of experiments to validate microfluidic mass transfer model
- Modeled Burns – Ramshaw experiments

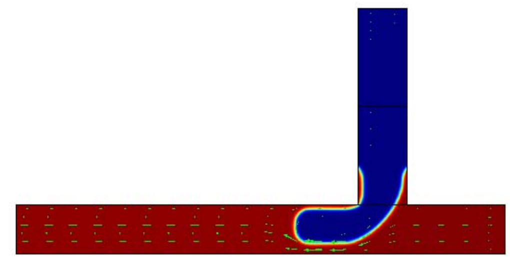
Initial Attempts to Model Experiments With COMSOL

Provides solutions that describe the interaction between multiple physical systems

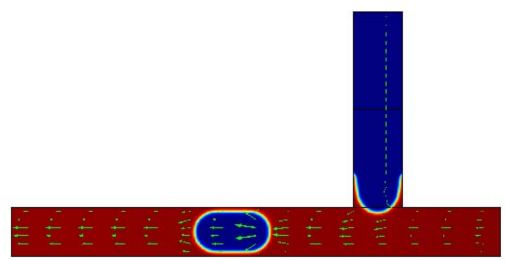
- Phase Field method
  - Provides improved phase conservation compared to Level Set
  - Mobility parameter allows matching of L/D of slugs



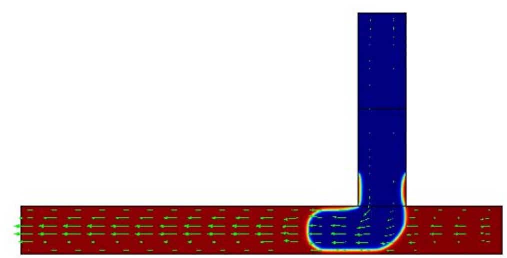
(a) Mobility Parameter = 10



(c) Mobility Parameter = 1000



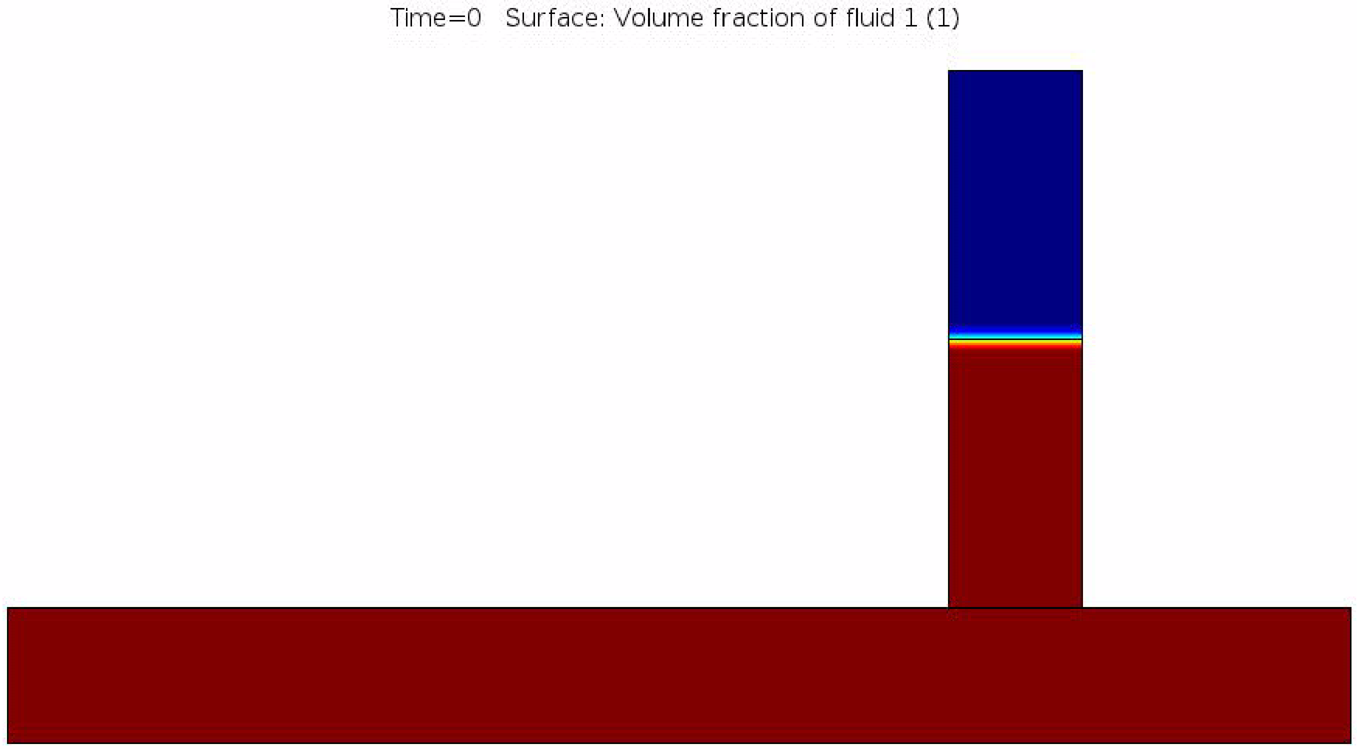
(b) Mobility Parameter = 100



(d) Mobility Parameter = 10,000

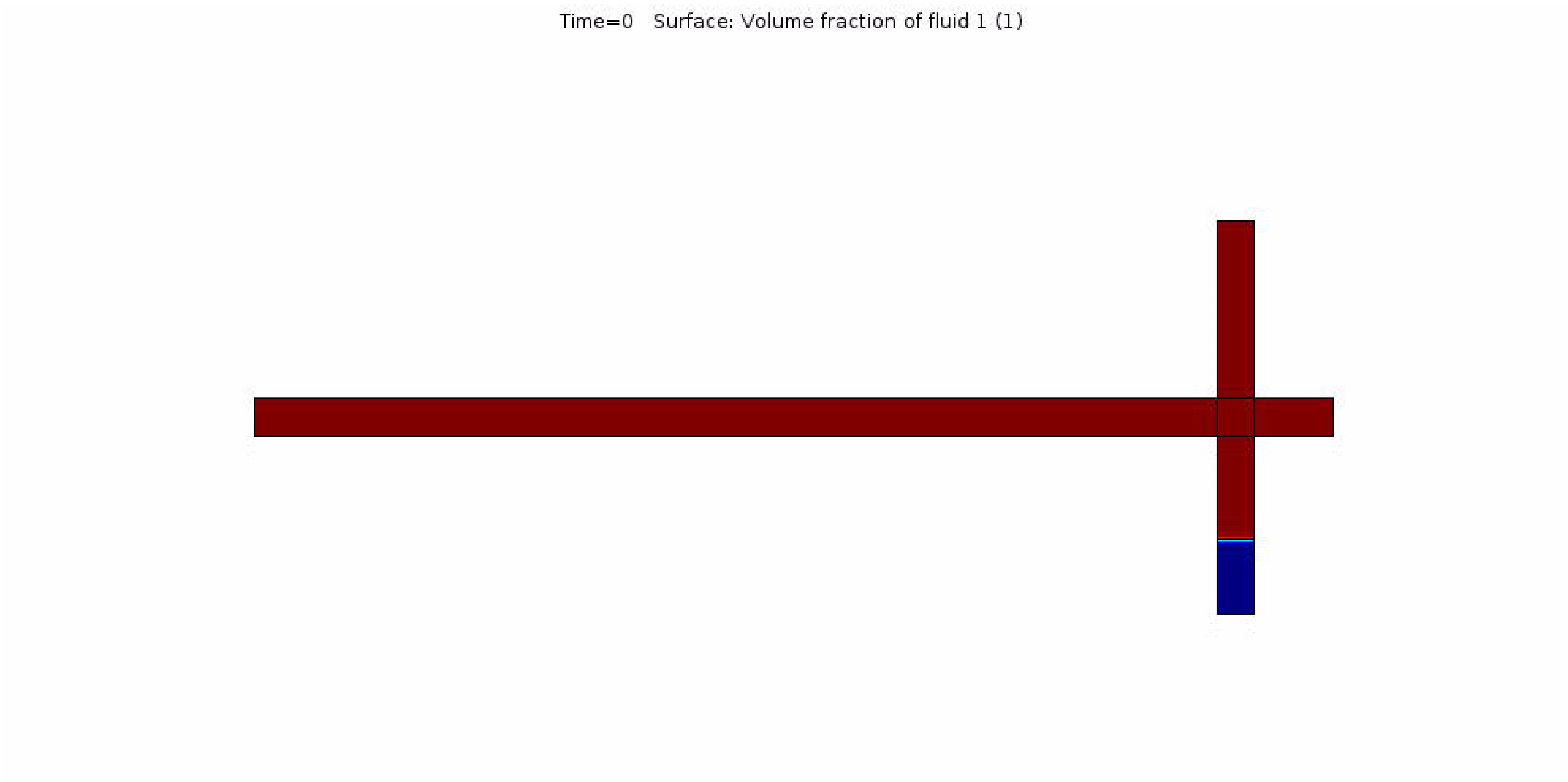
Initial Attempts to Model Experiments (Continued)

The dispersed phase can undergo spontaneous shrinkage with Cahn-Hilliard formulation in the Phase Field method



Initial Attempts to Model Experiments (Continued)

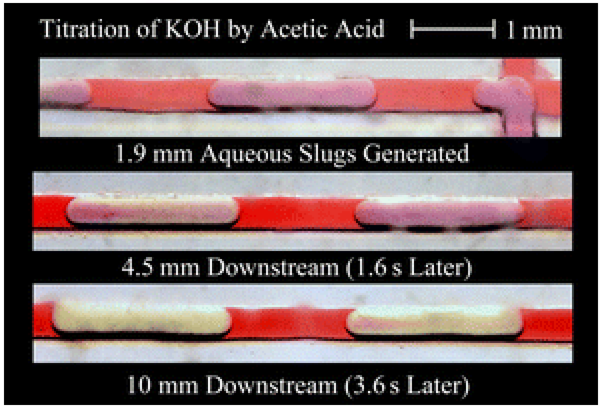
Spontaneous phase generation can also occur



COMSOL – Moving Mesh Method

- Uses an Arbitrary Lagrangian-Eulerian Formulation (ALE)
- Advantages
  - Phases are conserved
  - A discrete phase boundary allows specification of species locations and partition coefficient
  - Slug deformation based upon physical forces
- Disadvantage
  - Will not model formation of fluid slugs

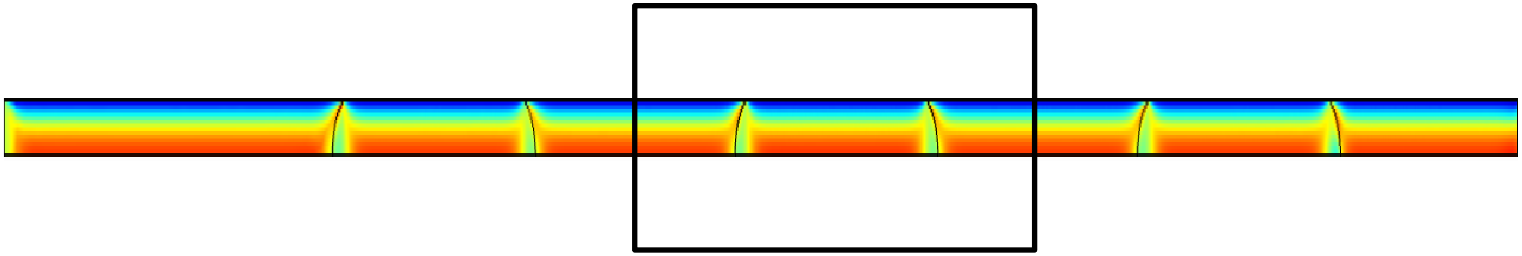
Case Study – Burns - Ramshaw Experiments



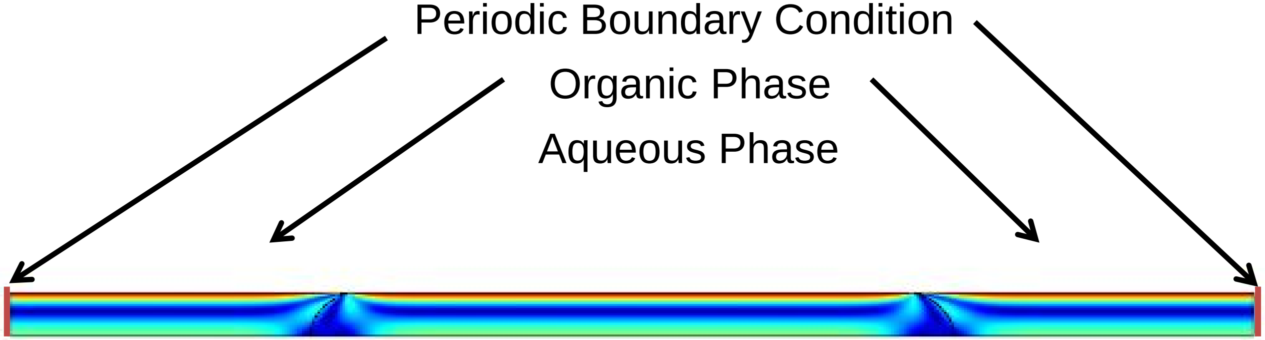
- Experimental conditions:
  - 0.38 mm square channel
  - Kerosene contains 0.5 M acetic acid
  - Water contains 0.25 M KOH
  - Flow velocity = 2.8 mm/sec
  - Acetic acid prefers aqueous phase
    (P =Co/Cw = 0.036)
- Modeled with moving mesh method
  - Contact angles modeled with Navier slip boundary condition
  - Distribution coefficient implemented with stiff spring method
  - Reaction between KOH and acetic acid modeled

Moving Mesh – Two step method

- Fluid dynamics is solved first

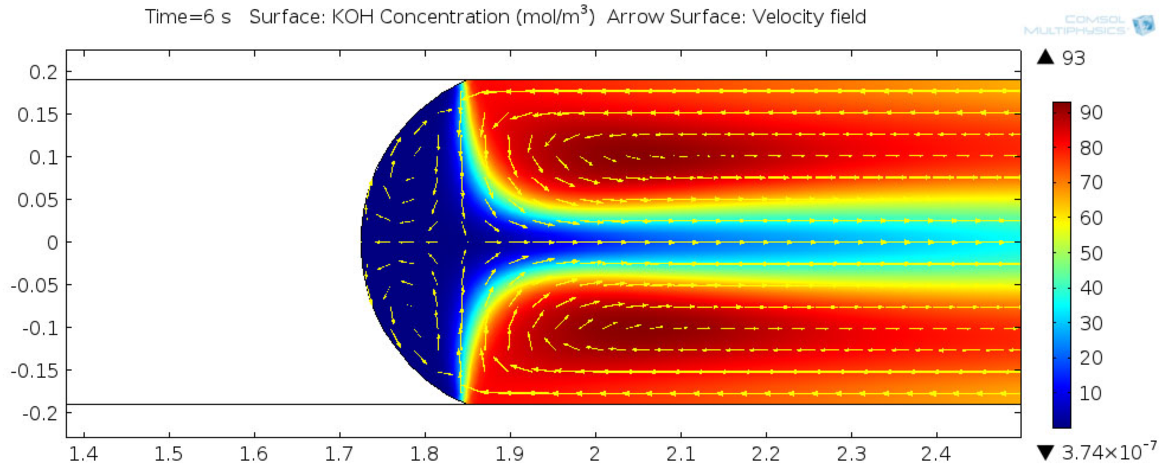


- Mass transfer solved under steady-state flow

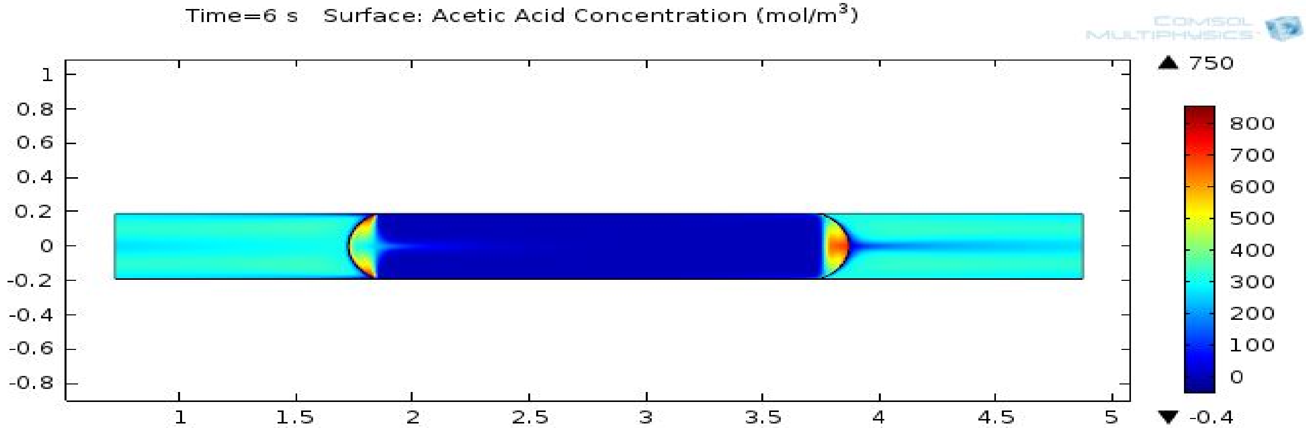


Characteristics of Flow at Interface

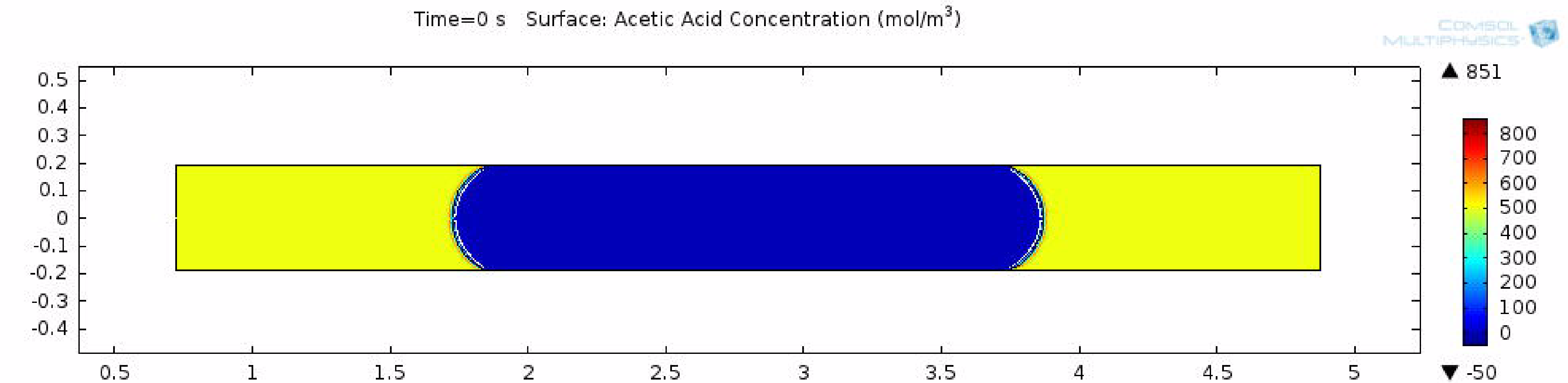
- Development of secondary flow pattern

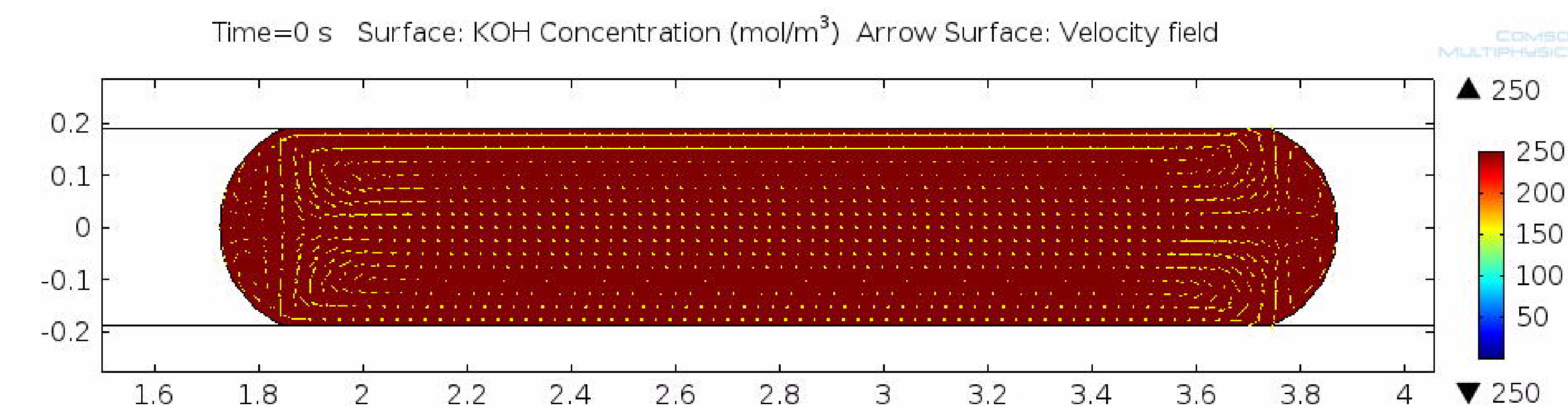


- Partition coefficient and inhibited mass transfer

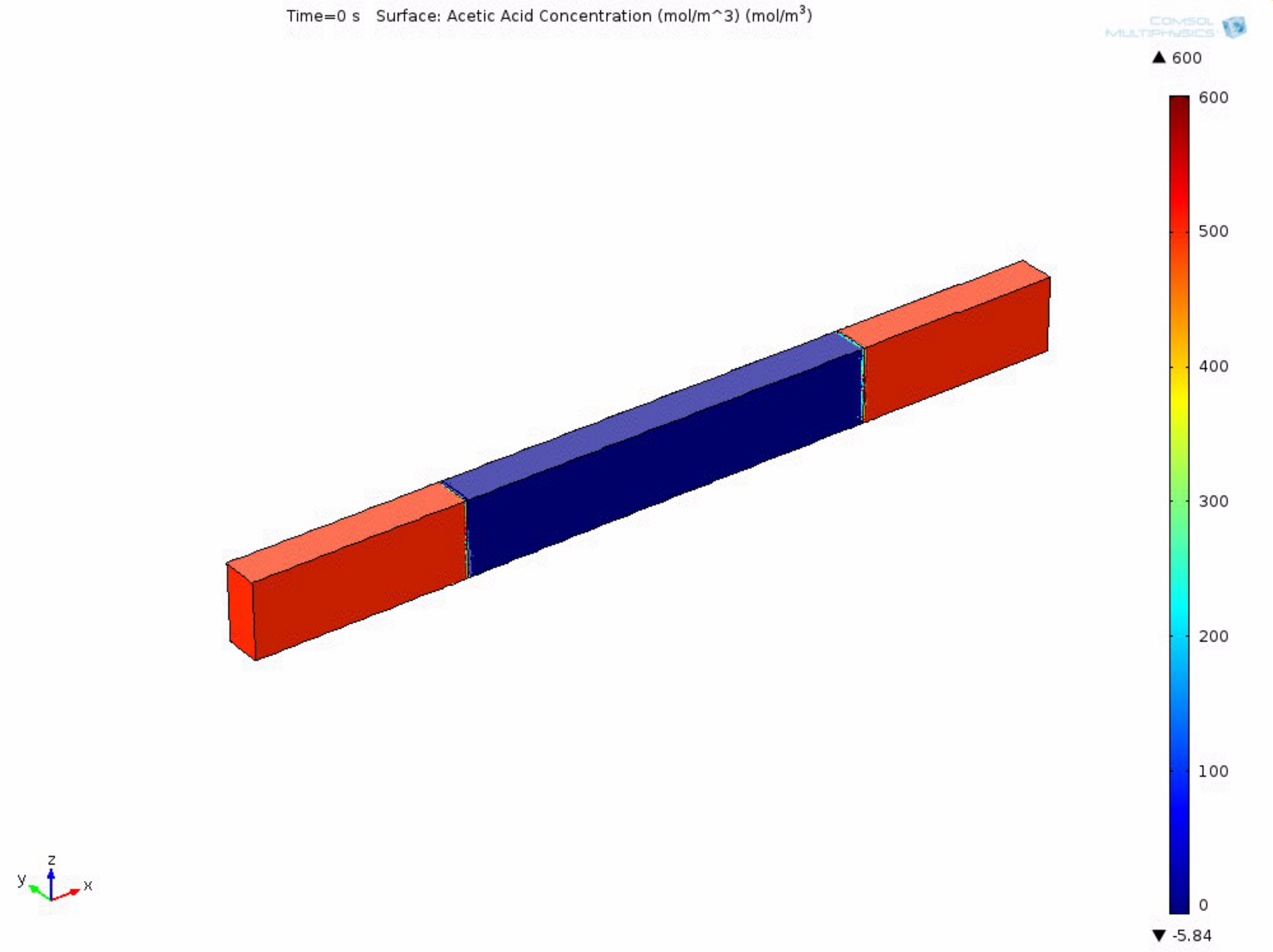


2D - Simulations

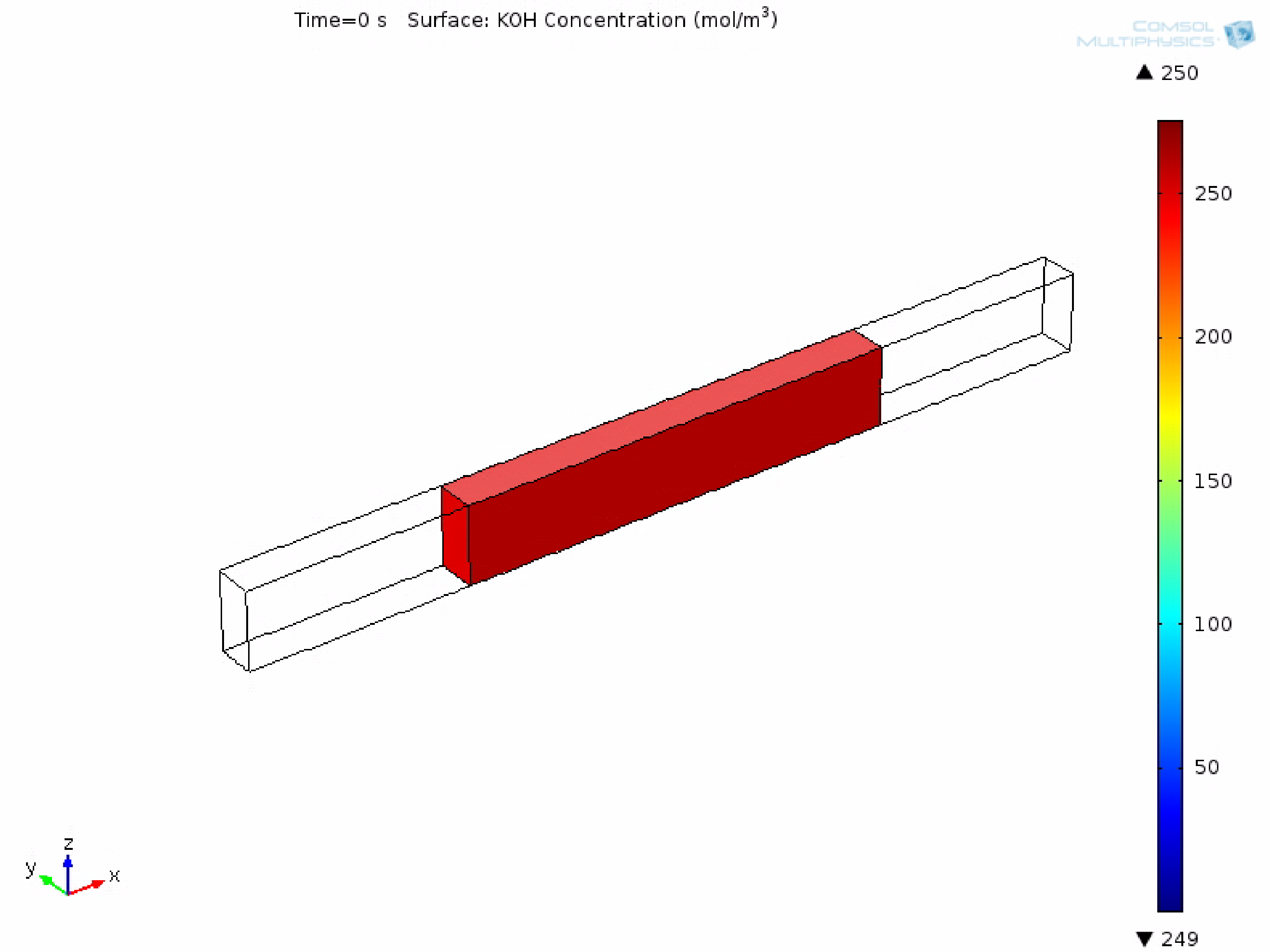




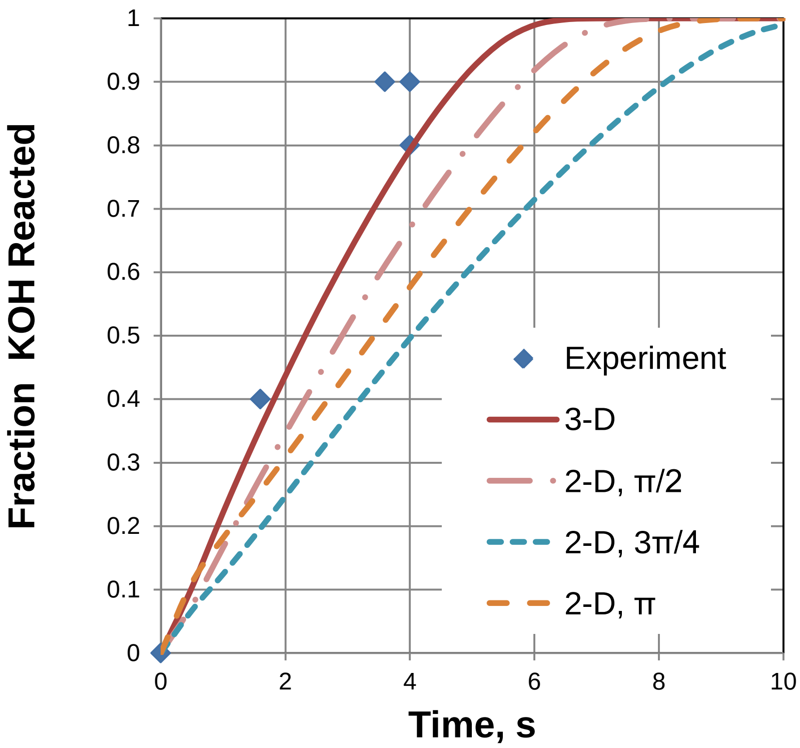
3D Simulation for Acetic Acid Concentration

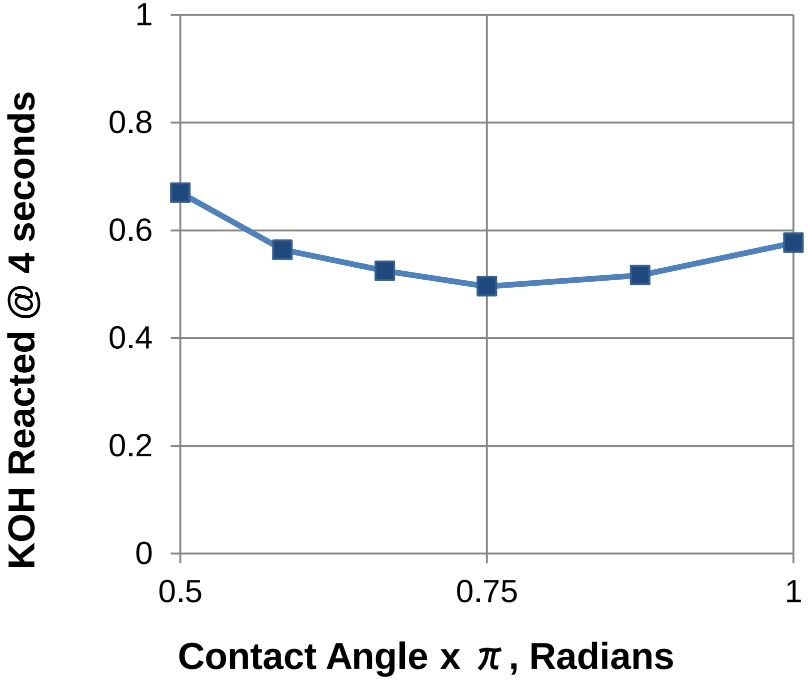


3D Simulation for Potassium Hydroxide Concentration



2D Contact Angle & 3D Model





Summary and Future Work

- Level set and Phase Field method model slug formation
  - Lack of discrete boundary creates challenge for mass transfer
- Moving mesh method
  - Does not model slug formation
  - Effectively models mass transfer
- Validated predictions provide basis for simulating experiments
- Improvement in 3-D re-meshing is needed to maintain element quality at contact angle $\neq \pi/2$